



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 21, 2024 – 12:27 am GMT

PDB ID : 7BBP  
Title : Crystal Structure of the second bromodomain of Pleckstrin homology domain interacting protein (PHIP) in complex with H4K5acK8ac  
Authors : Krojer, T.; Talon, R.; Fairhead, M.; Szykowska, A.; Burgess-Brown, N.A.; Brennan, P.E.; Arrowsmith, C.H.; Edwards, A.M.; Bountra, C.; von Delft, F.; Structural Genomics Consortium (SGC)  
Deposited on : 2020-12-18  
Resolution : 1.99 Å(reported)

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We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

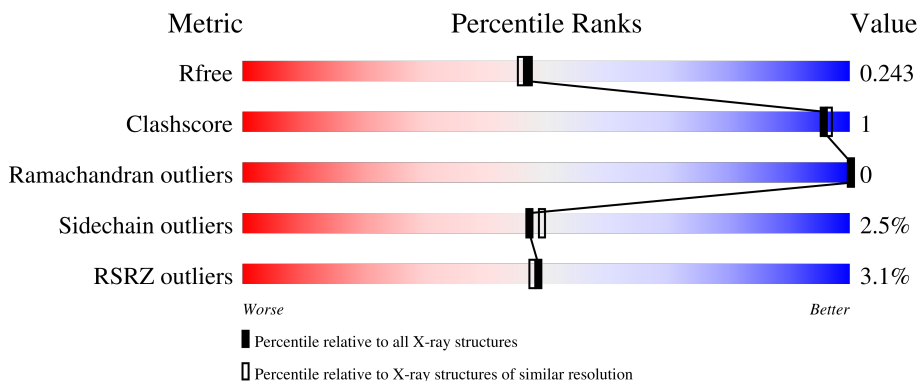
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

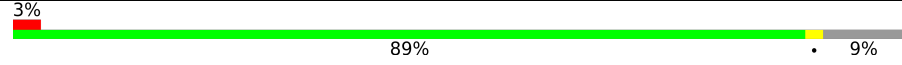
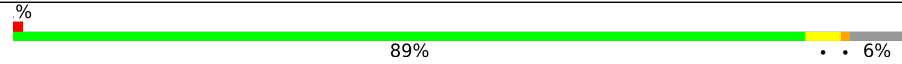
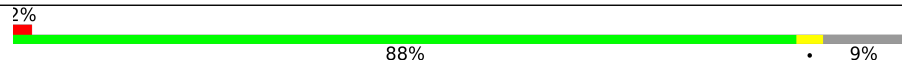

The reported resolution of this entry is 1.99 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



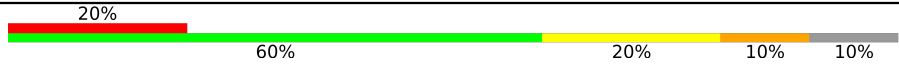

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AAA	128	
1	BBB	128	
1	CCC	128	
1	DDD	128	

*Continued on next page...*

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Mol	Chain	Length	Quality of chain
2	FFF	10	
2	GGG	10	

## 2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 4228 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called PH-interacting protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	AAA	117	980	624	160	189	7	0	1	0
1	BBB	120	1003	636	164	195	8	0	2	0
1	CCC	117	972	619	159	188	6	0	0	0
1	DDD	117	972	619	159	188	6	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	1313	SER	-	expression tag	UNP Q8WWQ0
AAA	1314	MET	-	expression tag	UNP Q8WWQ0
BBB	1313	SER	-	expression tag	UNP Q8WWQ0
BBB	1314	MET	-	expression tag	UNP Q8WWQ0
CCC	1313	SER	-	expression tag	UNP Q8WWQ0
CCC	1314	MET	-	expression tag	UNP Q8WWQ0
DDD	1313	SER	-	expression tag	UNP Q8WWQ0
DDD	1314	MET	-	expression tag	UNP Q8WWQ0

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	FFF	9	65	39	14	12	0	0	0
2	GGG	8	59	36	13	10	0	0	0

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	AAA	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula:  $C_2H_3O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	BBB	1	Total	C	O	0	0
			4	2	2		
4	CCC	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	AAA	38	Total 38	O 38	0	0
5	BBB	48	Total 48	O 48	0	0
5	CCC	35	Total 35	O 35	0	0
5	DDD	30	Total 30	O 30	0	0
5	FFF	7	Total 7	O 7	0	0
5	GGG	7	Total 7	O 7	0	0

### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

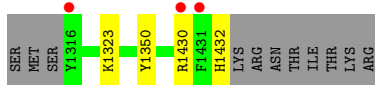
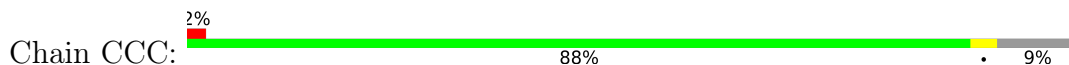
- Molecule 1: PH-interacting protein



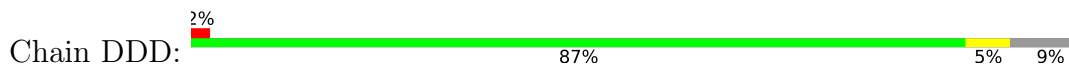
- Molecule 1: PH-interacting protein



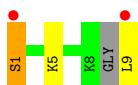
- Molecule 1: PH-interacting protein



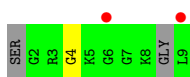
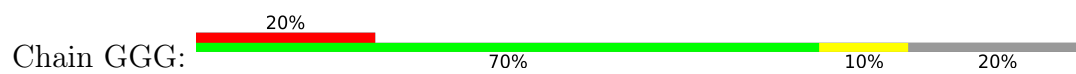
- Molecule 1: PH-interacting protein



- Molecule 2: Histone H4



- Molecule 2: Histone H4





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	69.21Å 58.31Å 77.12Å 90.00° 99.08° 90.00°	Depositor
Resolution (Å)	55.39 – 1.99 55.39 – 1.99	Depositor EDS
% Data completeness (in resolution range)	98.9 (55.39-1.99) 98.9 (55.39-1.99)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.93 (at 1.98Å)	Xtrriage
Refinement program	REFMAC 5.8.0267	Depositor
R, $R_{free}$	0.205 , 0.240 0.214 , 0.243	Depositor DCC
$R_{free}$ test set	2016 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	33.4	Xtrriage
Anisotropy	0.054	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 41.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	4228	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.36% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ALY, EDO, ACT

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	AAA	0.72	0/1003	0.73	0/1354
1	BBB	0.77	0/1026	0.75	1/1385 (0.1%)
1	CCC	0.75	0/995	0.73	0/1344
1	DDD	0.73	0/995	0.76	0/1344
2	FFF	1.43	1/38 (2.6%)	1.28	0/44
2	GGG	1.00	0/32	1.21	0/36
All	All	0.75	1/4089 (0.0%)	0.75	1/5507 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	FFF	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	FFF	1	SER	N-CA	6.20	1.58	1.46

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	BBB	1352	ASP	CB-CG-OD2	-5.13	113.69	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	FFF	1	SER	Peptide

## 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AAA	980	0	946	4	0
1	BBB	1003	0	962	3	0
1	CCC	972	0	938	1	0
1	DDD	972	0	938	1	0
2	FFF	65	0	71	2	0
2	GGG	59	0	62	1	0
3	AAA	4	0	6	3	0
4	BBB	4	0	3	0	0
4	CCC	4	0	3	0	0
5	AAA	38	0	0	0	0
5	BBB	48	0	0	0	0
5	CCC	35	0	0	0	0
5	DDD	30	0	0	0	0
5	FFF	7	0	0	0	0
5	GGG	7	0	0	1	0
All	All	4228	0	3929	9	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

The worst 5 of 9 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:GGG:4:GLY:O	5:GGG:101:HOH:O	2.16	0.60
1:DDD:1422:LEU:O	1:DDD:1426:LYS:HG2	2.07	0.54
1:AAA:1360:PRO:HB2	3:AAA:1501:EDO:C1	2.39	0.53
1:AAA:1360:PRO:HB2	3:AAA:1501:EDO:H12	1.94	0.49
1:AAA:1387:LEU:HD22	1:BBB:1386:ARG:CZ	2.46	0.45

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AAA	116/128 (91%)	116 (100%)	0	0	100	100
1	BBB	120/128 (94%)	120 (100%)	0	0	100	100
1	CCC	115/128 (90%)	115 (100%)	0	0	100	100
1	DDD	115/128 (90%)	115 (100%)	0	0	100	100
2	FFF	5/10 (50%)	5 (100%)	0	0	100	100
2	GGG	4/10 (40%)	4 (100%)	0	0	100	100
All	All	475/532 (89%)	475 (100%)	0	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AAA	111/121 (92%)	110 (99%)	1 (1%)	78	83
1	BBB	114/121 (94%)	111 (97%)	3 (3%)	46	48
1	CCC	110/121 (91%)	107 (97%)	3 (3%)	44	46
1	DDD	110/121 (91%)	106 (96%)	4 (4%)	35	34
2	FFF	3/3 (100%)	3 (100%)	0	100	100
2	GGG	2/3 (67%)	2 (100%)	0	100	100
All	All	450/490 (92%)	439 (98%)	11 (2%)	47	51

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	DDD	1408	LEU
1	DDD	1430	ARG
1	DDD	1432	HIS
1	DDD	1431	PHE
1	CCC	1323	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

4 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	ALY	GGG	5	2	10,11,12	0.52	0	7,12,14	0.53	0
2	ALY	FFF	5	2	10,11,12	0.59	0	7,12,14	0.36	0
2	ALY	FFF	8	2	10,11,12	0.42	0	7,12,14	0.65	0
2	ALY	GGG	8	2	10,11,12	0.50	0	7,12,14	0.68	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ALY	GGG	5	2	-	1/9/10/12	-
2	ALY	FFF	5	2	-	4/9/10/12	-
2	ALY	FFF	8	2	-	0/9/10/12	-
2	ALY	GGG	8	2	-	1/9/10/12	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	FFF	5	ALY	O-C-CA-CB
2	GGG	5	ALY	O-C-CA-CB
2	GGG	8	ALY	C-CA-CB-CG
2	FFF	5	ALY	CG-CD-CE-NZ
2	FFF	5	ALY	CA-CB-CG-CD

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	FFF	5	ALY	1	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

3 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	ACT	CCC	1501	-	3,3,3	1.07	0	3,3,3	0.70	0
4	ACT	BBB	1501	-	3,3,3	1.11	0	3,3,3	0.73	0
3	EDO	AAA	1501	-	3,3,3	0.13	0	2,2,2	0.60	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	AAA	1501	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	AAA	1501	EDO	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	AAA	1501	EDO	3	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	AAA	117/128 (91%)	-0.06	4 (3%) 45 44	24, 38, 62, 96	0
1	BBB	120/128 (93%)	-0.08	1 (0%) 86 85	23, 33, 53, 83	0
1	CCC	117/128 (91%)	-0.06	3 (2%) 56 54	21, 36, 75, 111	0
1	DDD	117/128 (91%)	0.13	3 (2%) 56 54	26, 43, 70, 97	0
2	FFF	7/10 (70%)	0.65	2 (28%) 0 0	27, 32, 51, 61	0
2	GGG	6/10 (60%)	1.06	2 (33%) 0 0	35, 49, 68, 69	0
All	All	484/532 (90%)	0.01	15 (3%) 49 48	21, 37, 70, 111	0

The worst 5 of 15 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	1316	TYR	4.2
1	CCC	1431	PHE	4.2
1	DDD	1431	PHE	3.9
1	DDD	1430	ARG	3.3
2	FFF	9	LEU	3.2

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	ALY	GGG	5	12/13	0.91	0.12	34,38,56,56	0
2	ALY	FFF	8	12/13	0.93	0.10	26,31,40,41	0
2	ALY	GGG	8	12/13	0.95	0.12	31,34,51,54	0
2	ALY	FFF	5	12/13	0.97	0.11	26,28,32,32	0



### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	ACT	CCC	1501	4/4	0.86	0.15	66,67,68,69	0
4	ACT	BBB	1501	4/4	0.93	0.16	55,56,57,59	0
3	EDO	AAA	1501	4/4	0.93	0.23	41,51,52,58	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.